



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 07:46 PM UTC

PDB ID : 5MJP / pdb_00005mjp
Title : Multi-bunch pink beam serial crystallography: Phycocyanin (One chip)
Authors : Meents, A.; Oberthuer, D.; Lieske, J.; Srajer, V.; Sarrou, I.
Deposited on : 2016-12-01
Resolution : 2.11 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

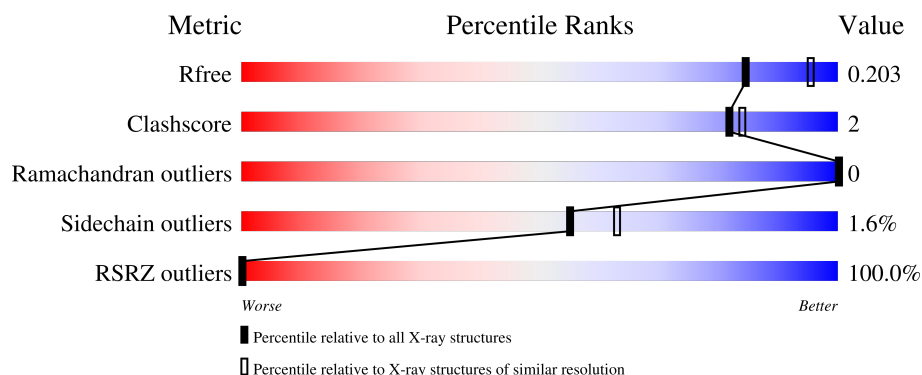
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	162	100% 94%6%
2	B	172	99% 95%5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MEN	B	72	-	-	-	X
3	CYC	A	501	-	-	-	X
3	CYC	B	201	-	-	-	X
3	CYC	B	202	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5431 atoms, of which 2604 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

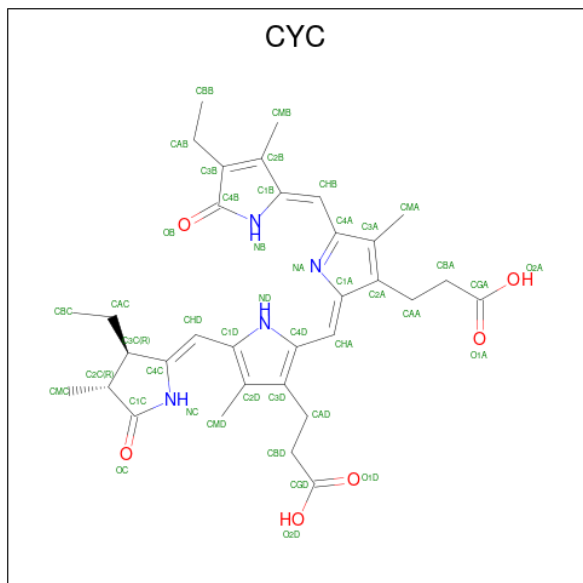
- Molecule 1 is a protein called C-phycocyanin alpha chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	162	Total	C	H	N	O	S	0	2	0
			2452	777	1216	209	243	7			

- Molecule 2 is a protein called C-phycocyanin beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	172	Total	C	H	N	O	S	0	2	0
			2559	794	1277	229	251	8			

- Molecule 3 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: $C_{33}H_{40}N_4O_6$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O		0	0
			80	33	37	4	6			
3	B	1	Total	C	H	N	O		0	0
			80	33	37	4	6			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	H	N	O	0	0
			80	33	37	4	6		

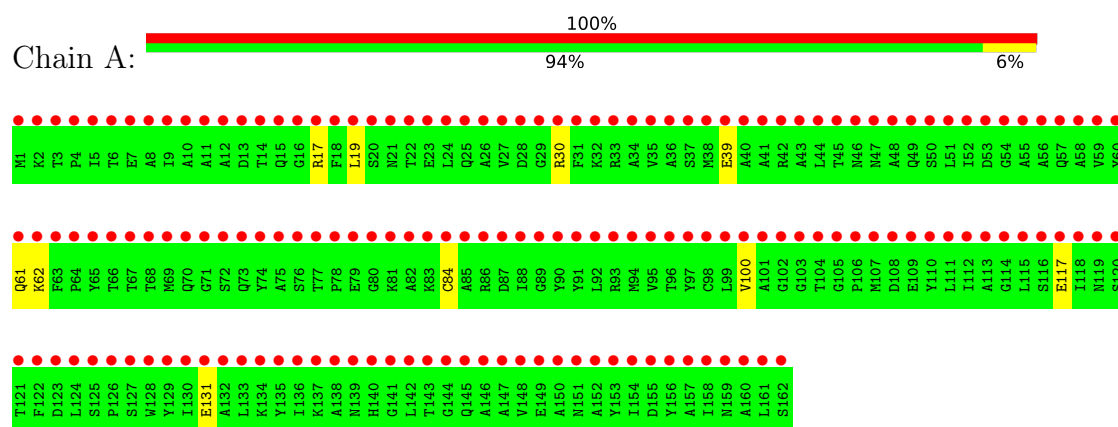
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	91	Total	O	0	0
			91	91		
4	B	89	Total	O	0	0
			89	89		

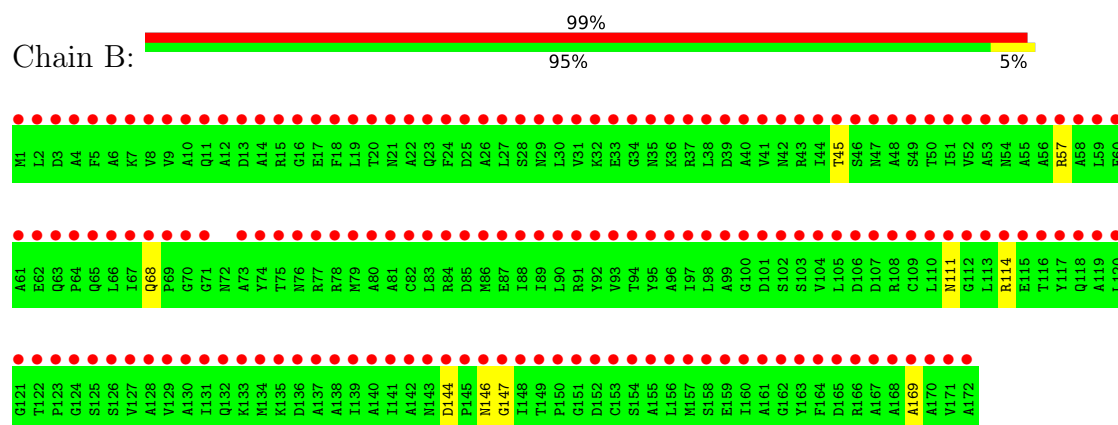
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: C-phycocyanin alpha chain



• Molecule 2: C-phycocyanin beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	187.80Å 187.80Å 60.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.90 – 2.11 14.90 – 2.11	Depositor EDS
% Data completeness (in resolution range)	65.3 (14.90-2.11) 65.5 (14.90-2.11)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.98 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.169 , 0.200 0.171 , 0.203	Depositor DCC
R_{free} test set	1533 reflections (6.47%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.35	EDS
Total number of atoms	5431	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CYC, MEN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.16	0/1270	0.29	0/1721
2	B	0.15	0/1292	0.29	0/1748
All	All	0.15	0/2562	0.29	0/3469

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1236	1216	1206	7	0
2	B	1282	1277	1282	6	0
3	A	43	37	37	2	0
3	B	86	74	73	0	0
4	A	91	0	0	3	2
4	B	89	0	0	4	1
All	All	2827	2604	2598	13	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (13) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLN:NE2	4:A:601:HOH:O	2.06	0.87
2:B:68[B]:GLN:OE1	4:B:601:HOH:O	2.05	0.74
1:A:39:GLU:OE1	4:A:602:HOH:O	2.12	0.67
2:B:144:ASP:OD1	4:B:602:HOH:O	2.14	0.66
1:A:131:GLU:OE1	4:A:603:HOH:O	2.18	0.56
3:A:501:CYC:HBC2	3:A:501:CYC:HMC1	1.89	0.55
1:A:84:CYS:HA	3:A:501:CYC:HHD	1.88	0.54
2:B:57:ARG:NH1	4:B:610:HOH:O	2.46	0.48
2:B:114:ARG:NH2	2:B:169:ALA:O	2.47	0.48
1:A:30:ARG:NH2	1:A:100:VAL:O	2.50	0.44
1:A:19:LEU:O	2:B:45:THR:HG21	2.18	0.43
1:A:17[B]:ARG:CZ	1:A:17[B]:ARG:HB3	2.49	0.42
2:B:147:GLY:O	4:B:603:HOH:O	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:677:HOH:O	4:A:677:HOH:O[6_556]	1.77	0.43
4:A:647:HOH:O	4:B:672:HOH:O[5_556]	2.04	0.16

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	162/162 (100%)	160 (99%)	2 (1%)	0	100	100
2	B	171/172 (99%)	169 (99%)	2 (1%)	0	100	100
All	All	333/334 (100%)	329 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	125/123 (102%)	123 (98%)	2 (2%)	55	63
2	B	129/127 (102%)	127 (98%)	2 (2%)	55	63
All	All	254/250 (102%)	250 (98%)	4 (2%)	55	63

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	LYS
1	A	117	GLU
2	B	111	ASN
2	B	146	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	139	ASN
2	B	42	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MEN	B	72	2	7,8,9	0.96	0	4,9,11	0.53	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	B	72	2	-	2/7/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	72	MEN	CA-CB-CG-OD1
2	B	72	MEN	CA-CB-CG-ND2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CYC	B	201	2	46,46,46	3.61	20 (43%)	63,67,67	1.80	15 (23%)
3	CYC	B	202	2	46,46,46	3.54	20 (43%)	63,67,67	1.68	12 (19%)
3	CYC	A	501	1	46,46,46	3.55	20 (43%)	63,67,67	1.76	17 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CYC	B	201	2	-	9/26/74/74	0/4/4/4
3	CYC	B	202	2	-	9/26/74/74	0/4/4/4
3	CYC	A	501	1	-	11/26/74/74	0/4/4/4

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	CYC	C1B-NB	9.40	1.53	1.37
3	B	202	CYC	C1B-NB	9.30	1.53	1.37
3	A	501	CYC	C1B-NB	9.23	1.53	1.37
3	B	202	CYC	C1C-NC	9.08	1.49	1.37
3	B	201	CYC	C1C-NC	8.94	1.49	1.37
3	A	501	CYC	C1C-NC	8.91	1.49	1.37
3	A	501	CYC	C4C-NC	7.72	1.52	1.37
3	B	202	CYC	C4C-NC	7.60	1.52	1.37
3	B	201	CYC	C4C-NC	7.58	1.52	1.37
3	B	201	CYC	C4B-NB	6.89	1.54	1.38
3	B	202	CYC	C4B-NB	6.82	1.53	1.38
3	A	501	CYC	C4B-NB	6.66	1.53	1.38
3	B	201	CYC	C1A-NA	6.24	1.52	1.38
3	B	201	CYC	CHD-C1D	6.03	1.54	1.40
3	A	501	CYC	C1A-NA	6.01	1.51	1.38
3	A	501	CYC	CHD-C1D	6.00	1.53	1.40
3	B	202	CYC	CHA-C4D	5.87	1.53	1.40
3	B	202	CYC	C1A-NA	5.86	1.51	1.38
3	B	201	CYC	CHA-C4D	5.84	1.53	1.40
3	B	201	CYC	CHB-C4A	5.83	1.54	1.40
3	B	201	CYC	C4A-NA	5.65	1.49	1.36
3	B	202	CYC	CHD-C1D	5.64	1.53	1.40
3	A	501	CYC	CHA-C4D	5.50	1.52	1.40
3	A	501	CYC	C4A-NA	5.42	1.48	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	CYC	CHB-C4A	5.42	1.53	1.40
3	B	202	CYC	C4A-NA	5.39	1.48	1.36
3	B	202	CYC	CHB-C4A	5.29	1.52	1.40
3	B	202	CYC	C1A-C2A	4.84	1.53	1.45
3	B	201	CYC	C2A-C3A	4.80	1.47	1.36
3	B	202	CYC	C2A-C3A	4.75	1.47	1.36
3	B	201	CYC	C1A-C2A	4.70	1.53	1.45
3	B	201	CYC	C2C-C1C	-4.67	1.47	1.52
3	A	501	CYC	C2A-C3A	4.64	1.46	1.36
3	A	501	CYC	C2C-C1C	-4.51	1.48	1.52
3	A	501	CYC	C1A-C2A	4.39	1.52	1.45
3	A	501	CYC	CHA-C1A	-4.06	1.31	1.38
3	B	202	CYC	C2C-C1C	-3.74	1.48	1.52
3	B	202	CYC	CHA-C1A	-3.62	1.31	1.38
3	B	201	CYC	CHA-C1A	-3.46	1.32	1.38
3	A	501	CYC	C4D-C3D	-3.10	1.35	1.42
3	B	201	CYC	C1B-C2B	2.70	1.49	1.45
3	B	202	CYC	CHD-C4C	-2.70	1.32	1.36
3	B	201	CYC	C4D-C3D	-2.69	1.36	1.42
3	A	501	CYC	OC-C1C	-2.66	1.18	1.23
3	B	201	CYC	C3B-C2B	2.65	1.42	1.36
3	B	202	CYC	OB-C4B	-2.62	1.18	1.23
3	B	202	CYC	C3B-C2B	2.60	1.42	1.36
3	A	501	CYC	OB-C4B	-2.59	1.18	1.23
3	A	501	CYC	CHB-C1B	-2.58	1.31	1.37
3	B	202	CYC	C1B-C2B	2.57	1.49	1.45
3	B	201	CYC	OC-C1C	-2.53	1.18	1.23
3	B	202	CYC	CHB-C1B	-2.51	1.31	1.37
3	A	501	CYC	C1B-C2B	2.48	1.49	1.45
3	A	501	CYC	C3B-C2B	2.46	1.42	1.36
3	B	202	CYC	C4D-C3D	-2.46	1.37	1.42
3	B	201	CYC	OB-C4B	-2.39	1.19	1.23
3	B	202	CYC	OC-C1C	-2.28	1.19	1.23
3	B	201	CYC	CHB-C1B	-2.17	1.32	1.37
3	A	501	CYC	CHD-C4C	-2.12	1.33	1.36
3	B	201	CYC	CHD-C4C	-2.11	1.33	1.36

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	CYC	C1C-NC-C4C	-4.98	107.16	113.41
3	B	201	CYC	C2C-C3C-C4C	4.52	108.12	101.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	CYC	C3C-C4C-NC	-4.40	102.28	107.94
3	B	202	CYC	C1C-NC-C4C	-4.30	108.02	113.41
3	B	201	CYC	C1C-NC-C4C	-3.96	108.44	113.41
3	B	202	CYC	C2C-C3C-C4C	3.68	106.86	101.34
3	B	202	CYC	CHA-C4D-C3D	3.67	135.11	127.22
3	B	202	CYC	CHA-C4D-ND	-3.58	117.20	125.29
3	B	202	CYC	C1D-CHD-C4C	-3.48	121.83	127.76
3	B	201	CYC	CMD-C2D-C1D	3.48	130.67	125.62
3	B	202	CYC	C2A-C1A-NA	-3.36	105.29	110.04
3	B	201	CYC	C2A-C1A-NA	-3.35	105.30	110.04
3	B	201	CYC	CHD-C4C-NC	3.34	129.80	125.63
3	B	201	CYC	C1B-C2B-C3B	3.27	111.23	107.86
3	B	202	CYC	C1B-NB-C4B	-3.15	106.79	110.66
3	B	201	CYC	CHA-C4D-C3D	3.14	133.96	127.22
3	B	201	CYC	CHA-C4D-ND	-3.13	118.21	125.29
3	B	201	CYC	CHA-C1A-NA	3.11	131.13	124.60
3	A	501	CYC	CHA-C1A-NA	3.06	131.02	124.60
3	A	501	CYC	C1B-NB-C4B	-3.05	106.92	110.66
3	A	501	CYC	C1D-CHD-C4C	-2.97	122.69	127.76
3	B	202	CYC	C1A-C2A-C3A	2.91	109.88	106.73
3	A	501	CYC	C2A-C1A-NA	-2.82	106.05	110.04
3	A	501	CYC	CMA-C3A-C4A	2.81	129.47	125.10
3	B	201	CYC	C1A-C2A-C3A	2.77	109.73	106.73
3	A	501	CYC	C1A-C2A-C3A	2.68	109.63	106.73
3	A	501	CYC	C1B-C2B-C3B	2.68	110.61	107.86
3	A	501	CYC	CHA-C4D-ND	-2.65	119.29	125.29
3	B	202	CYC	C1B-C2B-C3B	2.63	110.57	107.86
3	B	202	CYC	CHA-C1A-NA	2.52	129.89	124.60
3	B	201	CYC	C1B-NB-C4B	-2.50	107.59	110.66
3	A	501	CYC	C1B-CHB-C4A	-2.44	122.06	128.06
3	A	501	CYC	CHA-C4D-C3D	2.38	132.33	127.22
3	A	501	CYC	CAD-C3D-C4D	-2.30	122.12	125.77
3	B	201	CYC	CMC-C2C-C1C	-2.30	107.45	112.40
3	A	501	CYC	CMD-C2D-C1D	2.29	128.95	125.62
3	A	501	CYC	O2D-CGD-CBD	2.26	121.13	114.00
3	B	201	CYC	CAB-C3B-C4B	2.23	124.82	121.37
3	A	501	CYC	CAB-C3B-C4B	2.23	124.82	121.37
3	B	201	CYC	O2A-CGA-CBA	2.18	120.89	114.00
3	B	202	CYC	CAB-C3B-C4B	2.18	124.74	121.37
3	B	201	CYC	C1B-CHB-C4A	-2.12	122.84	128.06
3	B	202	CYC	C1B-CHB-C4A	-2.10	122.90	128.06
3	A	501	CYC	CBC-CAC-C3C	-2.08	108.99	113.41

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	CYC	NA-C4A-CHB-C1B
3	A	501	CYC	C3A-C4A-CHB-C1B
3	A	501	CYC	C4C-C3C-CAC-CBC
3	A	501	CYC	NC-C4C-CHD-C1D
3	B	201	CYC	NA-C4A-CHB-C1B
3	B	201	CYC	C3A-C4A-CHB-C1B
3	B	202	CYC	NA-C4A-CHB-C1B
3	B	202	CYC	C3A-C4A-CHB-C1B
3	B	202	CYC	C2C-C3C-CAC-CBC
3	B	202	CYC	C4C-C3C-CAC-CBC
3	B	201	CYC	C2B-C3B-CAB-CBB
3	A	501	CYC	ND-C1D-CHD-C4C
3	B	202	CYC	ND-C1D-CHD-C4C
3	B	201	CYC	C2D-C1D-CHD-C4C
3	B	202	CYC	C2D-C1D-CHD-C4C
3	B	201	CYC	ND-C1D-CHD-C4C
3	A	501	CYC	C2D-C1D-CHD-C4C
3	B	201	CYC	C4B-C3B-CAB-CBB
3	A	501	CYC	C2B-C3B-CAB-CBB
3	A	501	CYC	C2C-C3C-CAC-CBC
3	A	501	CYC	CAA-CBA-CGA-O2A
3	A	501	CYC	CAA-CBA-CGA-O1A
3	B	201	CYC	CAD-CBD-CGD-O2D
3	B	202	CYC	CAA-CBA-CGA-O2A
3	B	201	CYC	CAD-CBD-CGD-O1D
3	B	202	CYC	CAA-CBA-CGA-O1A
3	B	202	CYC	CAD-CBD-CGD-O2D
3	A	501	CYC	C4B-C3B-CAB-CBB
3	B	201	CYC	CAA-CBA-CGA-O2A

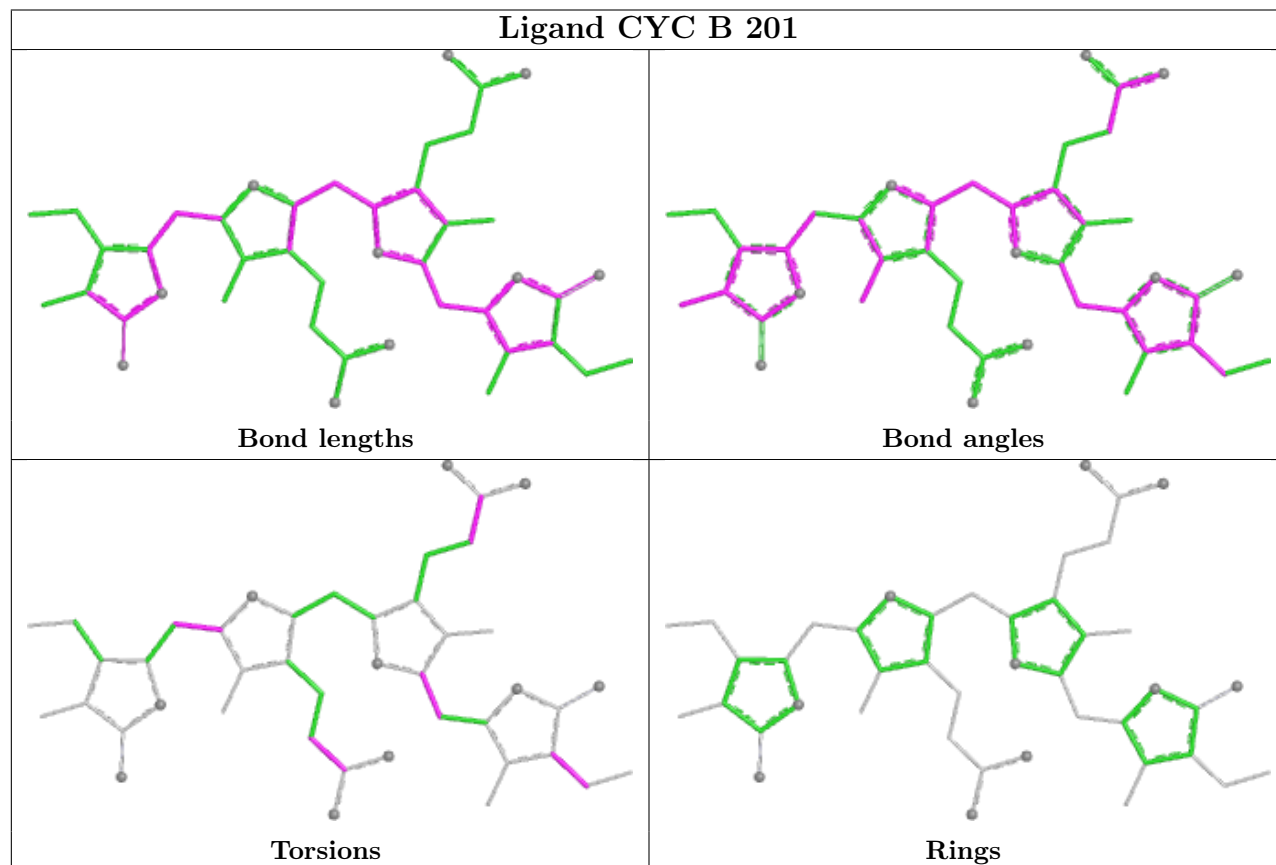
There are no ring outliers.

1 monomer is involved in 2 short contacts:

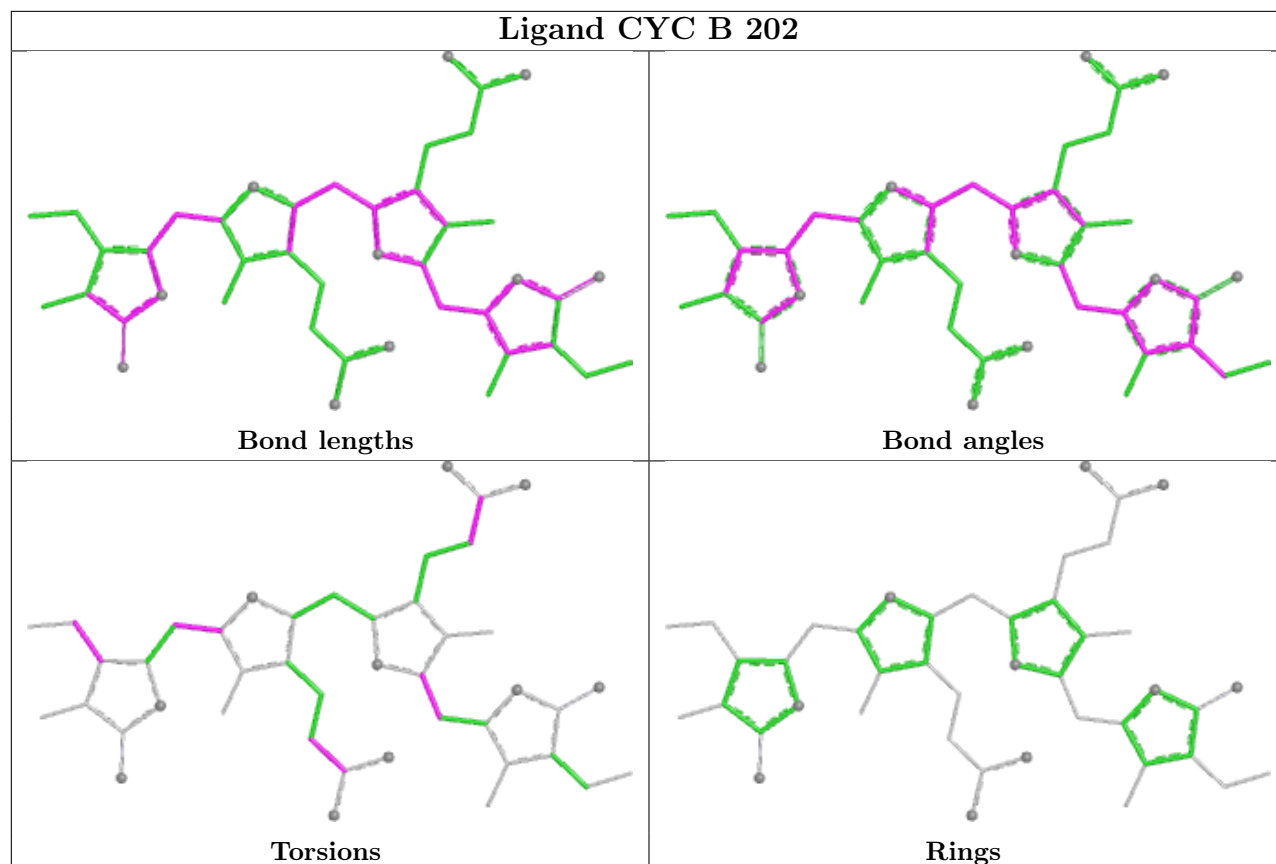
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	CYC	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

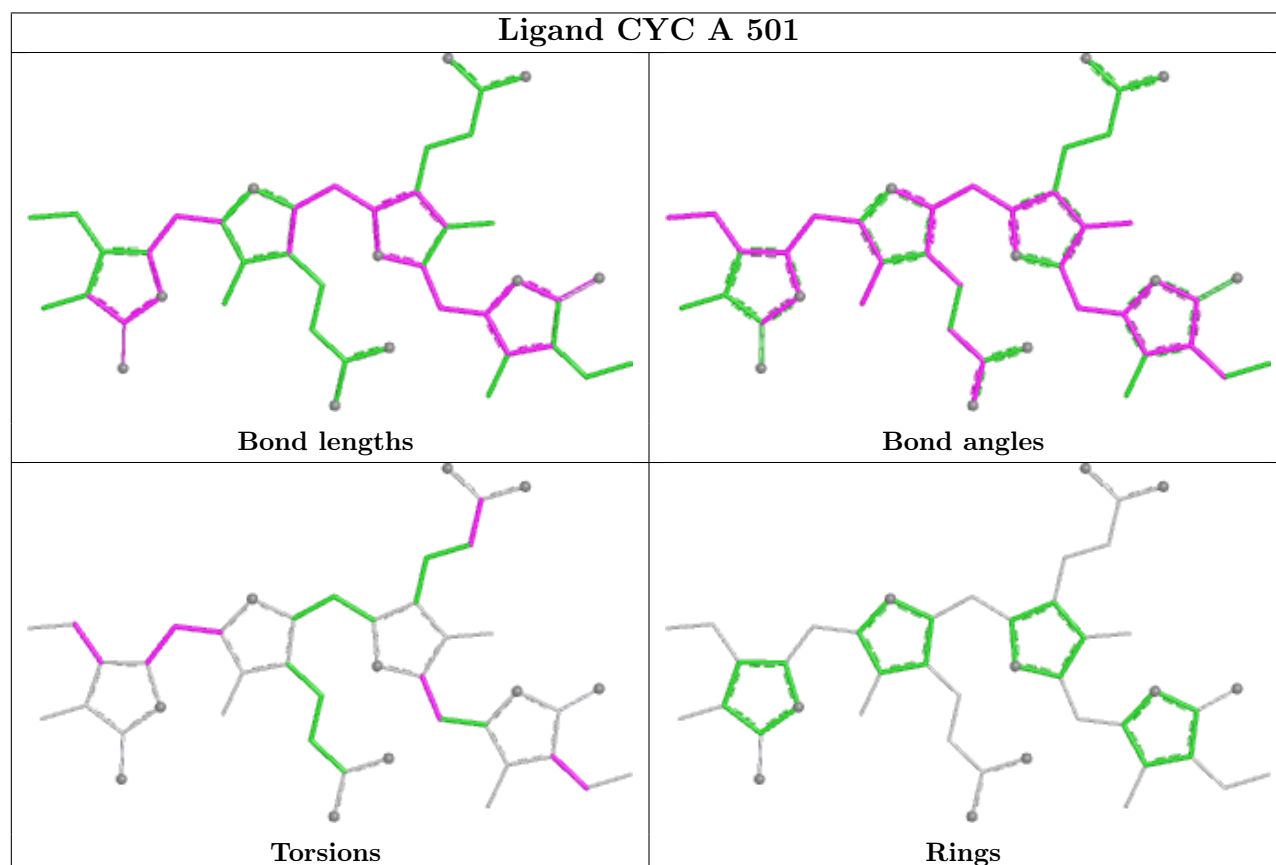
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand CYC B 202



Ligand CYC A 501



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	162/162 (100%)	10.42	162 (100%) 0 0	13, 21, 39, 61	1 (0%)
2	B	171/172 (99%)	12.33	171 (100%) 0 0	14, 27, 46, 61	2 (1%)
All	All	333/334 (99%)	11.40	333 (100%) 0 0	13, 24, 45, 61	3 (0%)

All (333) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	ALA	44.7
2	B	172	ALA	36.2
2	B	111	ASN	32.7
2	B	125	SER	28.5
2	B	150	PRO	28.4
2	B	144	ASP	28.0
2	B	110	LEU	26.4
2	B	142	ALA	25.9
2	B	151	GLY	23.6
2	B	116	THR	22.1
2	B	131	ILE	22.0
2	B	29	ASN	21.8
1	A	11	ALA	21.8
2	B	30	LEU	21.2
2	B	24	PHE	21.1
1	A	83	LYS	20.9
2	B	112	GLY	20.9
1	A	15	GLN	20.0
2	B	67	ILE	18.8
1	A	72	SER	18.6
2	B	154	SER	18.6
2	B	22	ALA	18.5
1	A	34	ALA	18.3
1	A	58	ALA	18.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	50	THR	18.0
1	A	42	ARG	18.0
1	A	81	LYS	17.6
1	A	46	ASN	17.4
1	A	70	GLN	17.1
2	B	149	THR	16.9
2	B	28	SER	16.8
2	B	32	LYS	16.7
1	A	64	PRO	16.7
2	B	117	TYR	16.7
2	B	105	LEU	16.6
1	A	37	SER	16.5
1	A	113	ALA	16.4
2	B	102	SER	16.0
2	B	54	ASN	16.0
1	A	118	ILE	15.9
2	B	108	ARG	15.9
2	B	146	ASN	15.9
2	B	36	LYS	15.6
2	B	120	LEU	15.5
1	A	57	GLN	15.3
1	A	45	THR	15.2
2	B	171	VAL	15.2
2	B	33	GLU	15.1
2	B	89	ILE	15.0
1	A	76	SER	15.0
2	B	15	ARG	15.0
2	B	160	ILE	14.9
2	B	156	LEU	14.5
2	B	87	GLU	14.5
2	B	5	PHE	14.5
2	B	1	MET	14.5
2	B	132	GLN	14.4
2	B	77	ARG	14.3
2	B	8	VAL	14.2
2	B	66	LEU	14.2
2	B	7	LYS	14.2
2	B	118	GLN	14.1
1	A	142	LEU	14.1
2	B	73	ALA	14.0
2	B	159	GLU	14.0
2	B	124	GLY	13.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	127	VAL	13.8
2	B	119	ALA	13.7
2	B	55	ALA	13.7
2	B	97	ILE	13.6
2	B	11	GLN	13.6
2	B	114	ARG	13.6
2	B	27	LEU	13.6
1	A	74	TYR	13.5
1	A	106	PRO	13.5
1	A	156	TYR	13.5
2	B	84	ARG	13.4
1	A	35	VAL	13.3
2	B	123	PRO	13.3
2	B	145	PRO	13.3
1	A	5	ILE	13.2
1	A	66	THR	13.1
1	A	109	GLU	13.1
1	A	120	SER	13.1
2	B	141	ILE	13.0
2	B	39	ASP	13.0
1	A	60	TYR	13.0
2	B	163	TYR	12.9
2	B	153	CYS	12.8
1	A	40	ALA	12.8
2	B	104	VAL	12.8
1	A	47	ASN	12.7
2	B	68[A]	GLN	12.7
1	A	8	ALA	12.7
1	A	31	PHE	12.7
2	B	113	LEU	12.7
2	B	148	ILE	12.7
1	A	116	SER	12.5
1	A	41	ALA	12.5
2	B	158	SER	12.5
2	B	164	PHE	12.5
1	A	32	LYS	12.5
1	A	150	ALA	12.4
1	A	87	ASP	12.4
1	A	79	GLU	12.3
2	B	57	ARG	12.3
1	A	29	GLY	12.2
2	B	65	GLN	12.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	19	LEU	12.2
1	A	9	ILE	12.1
1	A	77	THR	12.0
2	B	138	ALA	12.0
2	B	92	TYR	11.9
2	B	48	ALA	11.9
1	A	110	TYR	11.9
1	A	30	ARG	11.9
2	B	130	ALA	11.9
1	A	69	MET	11.9
2	B	133	LYS	11.8
1	A	128	TRP	11.8
1	A	39	GLU	11.7
1	A	139	ASN	11.7
2	B	155	ALA	11.7
2	B	42	ASN	11.7
2	B	170	ALA	11.6
1	A	78	PRO	11.6
2	B	147	GLY	11.6
1	A	17[A]	ARG	11.5
2	B	83	LEU	11.5
2	B	21	ASN	11.4
1	A	111	LEU	11.4
2	B	94	THR	11.4
1	A	130	ILE	11.4
2	B	31	VAL	11.4
2	B	162	GLY	11.3
2	B	69	PRO	11.3
1	A	28	ASP	11.2
2	B	109	CYS	11.2
2	B	95	TYR	11.2
1	A	135	TYR	11.2
1	A	138	ALA	11.1
1	A	27	VAL	11.1
1	A	159	ASN	11.1
2	B	52	VAL	11.0
2	B	63	GLN	11.0
2	B	107	ASP	11.0
2	B	10	ALA	11.0
2	B	75	THR	11.0
2	B	93	VAL	11.0
2	B	76	ASN	10.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	44	LEU	10.9
1	A	146	ALA	10.8
2	B	143	ASN	10.7
1	A	91	TYR	10.7
1	A	143	THR	10.7
2	B	81	ALA	10.7
2	B	136	ASP	10.6
2	B	2	LEU	10.5
1	A	94	MET	10.5
1	A	3	THR	10.5
1	A	22	THR	10.5
1	A	136	ILE	10.5
2	B	106	ASP	10.5
2	B	64	PRO	10.4
2	B	74	TYR	10.4
1	A	10	ALA	10.4
2	B	38	LEU	10.4
1	A	59	VAL	10.4
1	A	148	VAL	10.4
1	A	89	GLY	10.3
1	A	121	THR	10.3
2	B	161	ALA	10.3
1	A	123	ASP	10.3
2	B	129	VAL	10.3
1	A	124	LEU	10.3
2	B	17	GLU	10.3
1	A	153	TYR	10.3
2	B	61	ALA	10.3
1	A	100	VAL	10.2
1	A	140	HIS	10.2
2	B	135	LYS	10.2
1	A	125	SER	10.2
1	A	161	LEU	10.1
1	A	61	GLN	10.1
2	B	23	GLN	10.1
2	B	122	THR	10.1
2	B	128	ALA	10.0
1	A	114	GLY	9.9
1	A	1	MET	9.9
2	B	126	SER	9.9
2	B	100	GLY	9.9
2	B	139	ILE	9.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	90	TYR	9.9
2	B	91	ARG	9.9
2	B	115	GLU	9.8
2	B	62	GLU	9.8
1	A	129	TYR	9.8
2	B	14	ALA	9.7
2	B	165	ASP	9.7
2	B	166	ARG	9.7
2	B	51	ILE	9.6
1	A	53	ASP	9.6
1	A	14	THR	9.6
1	A	71	GLY	9.6
2	B	167	ALA	9.6
1	A	49	GLN	9.5
2	B	121	GLY	9.5
2	B	59	LEU	9.5
2	B	60	PHE	9.5
1	A	7	GLU	9.5
2	B	12	ALA	9.5
2	B	152	ASP	9.4
2	B	19	LEU	9.4
2	B	41	VAL	9.3
1	A	133	LEU	9.3
1	A	21	ASN	9.3
1	A	147	ALA	9.3
2	B	140	ALA	9.3
1	A	95	VAL	9.2
1	A	63	PHE	9.2
1	A	67	THR	9.2
2	B	85	ASP	9.1
2	B	26	ALA	9.0
1	A	84	CYS	9.0
1	A	68	THR	9.0
2	B	40	ALA	9.0
1	A	16	GLY	9.0
1	A	65	TYR	8.9
2	B	103	SER	8.9
2	B	25	ASP	8.9
1	A	6	THR	8.9
1	A	127	SER	8.8
2	B	49	SER	8.8
2	B	44	ILE	8.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	88	ILE	8.7
1	A	96	THR	8.7
1	A	137	LYS	8.7
1	A	122	PHE	8.7
1	A	75	ALA	8.6
1	A	88	ILE	8.5
1	A	62	LYS	8.5
1	A	52	ILE	8.5
1	A	13	ASP	8.5
1	A	51	LEU	8.5
1	A	2	LYS	8.4
2	B	46	SER	8.4
1	A	73	GLN	8.4
2	B	4	ALA	8.3
2	B	169	ALA	8.3
2	B	45	THR	8.2
1	A	25	GLN	8.1
1	A	93	ARG	8.1
1	A	112	ILE	8.0
2	B	157	MET	8.0
2	B	56	ALA	8.0
2	B	96	ALA	8.0
1	A	99	LEU	8.0
2	B	18	PHE	8.0
1	A	102	GLY	8.0
2	B	58	ALA	8.0
1	A	18[A]	PHE	8.0
2	B	9	VAL	8.0
2	B	90	LEU	8.0
1	A	48	ALA	7.9
2	B	137	ALA	7.9
2	B	16	GLY	7.9
1	A	24	LEU	7.9
2	B	98	LEU	7.8
2	B	99	ALA	7.8
2	B	47	ASN	7.8
2	B	53	ALA	7.7
1	A	141	GLY	7.7
2	B	70	GLY	7.7
1	A	119	ASN	7.7
2	B	35	ASN	7.7
1	A	144	GLY	7.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	55	ALA	7.6
1	A	82	ALA	7.6
1	A	85	ALA	7.6
1	A	38	MET	7.5
1	A	126	PRO	7.5
1	A	26	ALA	7.5
1	A	80	GLY	7.5
1	A	132	ALA	7.5
1	A	97	TYR	7.5
2	B	78	ARG	7.4
1	A	157	ALA	7.4
2	B	43	ARG	7.3
1	A	107	MET	7.3
2	B	6	ALA	7.3
1	A	33	ARG	7.2
2	B	168	ALA	7.2
1	A	152	ALA	7.2
1	A	92	LEU	7.1
1	A	115	LEU	7.1
2	B	20[A]	THR	7.1
1	A	158	ILE	7.0
1	A	20	SER	7.0
1	A	43	ALA	7.0
2	B	13	ASP	7.0
1	A	98	CYS	7.0
1	A	104	THR	6.8
2	B	3	ASP	6.8
2	B	80	ALA	6.8
1	A	12	ALA	6.8
1	A	155	ASP	6.8
1	A	56	ALA	6.7
1	A	117	GLU	6.7
2	B	134	MET	6.7
1	A	108	ASP	6.6
1	A	145	GLN	6.5
1	A	162	SER	6.5
1	A	151	ASN	6.3
2	B	34	GLY	6.2
2	B	71	GLY	6.2
1	A	134	LYS	6.1
1	A	23	GLU	6.0
2	B	86	MET	5.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	154	ILE	5.9
1	A	131	GLU	5.8
1	A	4	PRO	5.8
2	B	101	ASP	5.7
1	A	160	ALA	5.6
2	B	79	MET	5.6
1	A	50	SER	5.6
1	A	103	GLY	5.5
1	A	86	ARG	5.5
1	A	101	ALA	5.5
1	A	54	GLY	5.3
2	B	82	CYS	5.1
2	B	37	ARG	4.7
1	A	105	GLY	4.6
1	A	149	GLU	2.9

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MEN	B	72	9/10	0.44	0.67	26,42,59,59	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

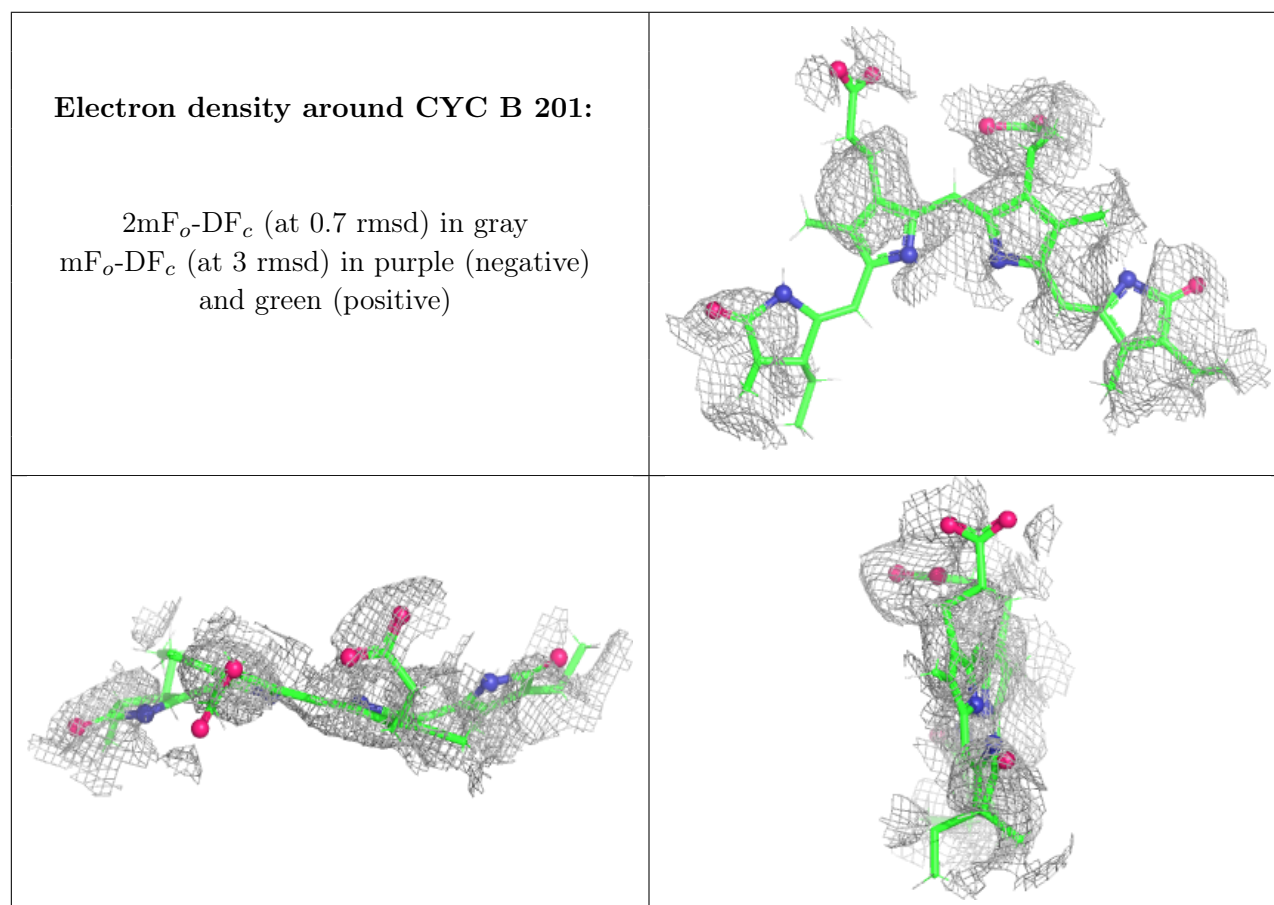
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CYC	B	201	43/43	0.24	0.59	25,34,63,64	0
3	CYC	B	202	43/43	0.24	0.65	21,29,39,40	0

Continued on next page...

Continued from previous page...

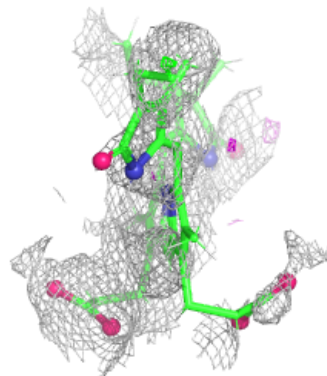
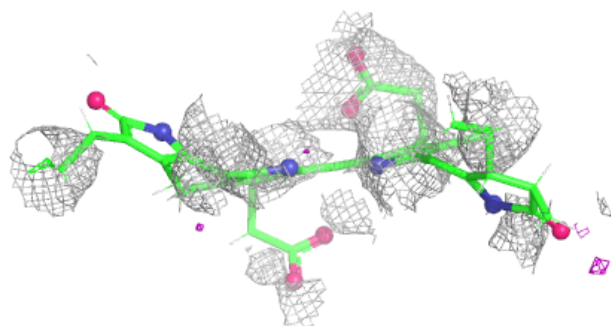
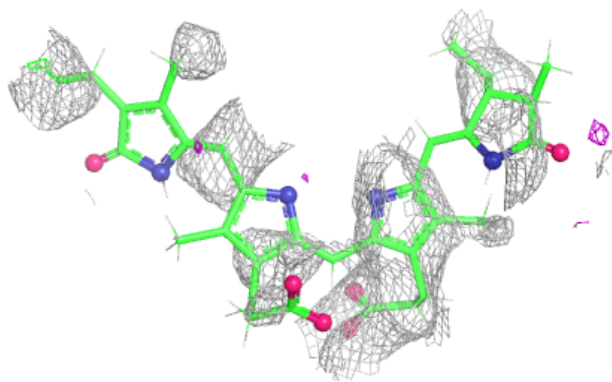
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CYC	A	501	43/43	0.40	0.47	12,17,24,28	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



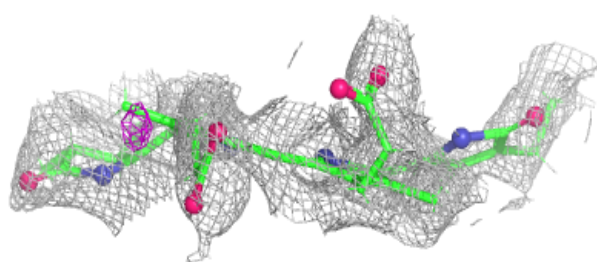
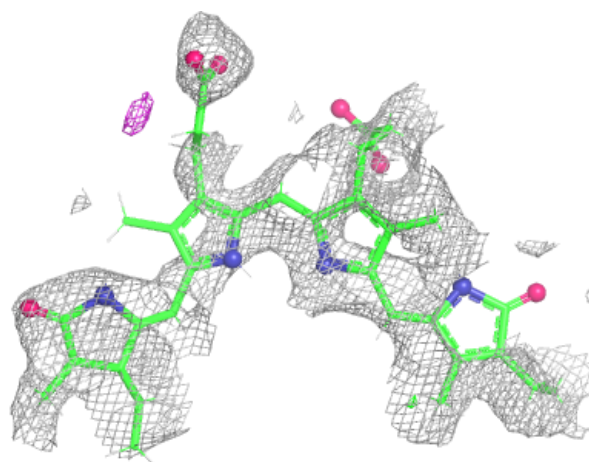
Electron density around CYC B 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CYC A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.